Prototyping by First Principles-Based Modeling: A Virtual Reactor

Methods Challenges and Computing Needs for a Comprehensive High Fidelity Model of a Nuclear Reactor

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Virtual Reactor Model: Why Resurrect an Old Idea

- KWU ~ 1977
- EG&G Idaho ~ 1988
- Numerical Reactor (ANL, Purdue, UIUC(?) etc) ~ now
- All had/have the approach of coupling codes

- Now and Future: Detailed Comprehensive Physical Models (Non-Linear) -- mimicking the reactors zones
- Evolving as Better Understanding of Underlying Physics is Achieved / Becomes more Amenable to Efficient Modeling

Objective: First Principles-Based Comprehensive Reactor Model

- Create reactor modeling capability for many possible applications
  - Design and Prototyping
  - Safety Characterization
  - Optimization
  - Fuel Cycle and Nonproliferation Characterization and Improvement
  - Etc …

Objective: First Principles-Based Comprehensive Reactor Model

- **Model Reactor in Detail with Level of Fidelity as High as Desired for Application being Considered**
- **Model to be based on a Hierarchy of sub-Models**
  - **Full Reactor Transport Theory Neutronics Treatment**
  - **Online Treatment/Preparation of Cross Sections/Nuclear Data**
  - **Explicit Detailed Treatment of Resonances in Diffuse and Lumped Fuels**
  - **Fully Tightly Coupled Thermal-Hydraulics (Multi-physics Approach)**
- **First Principles-Based Feedback Effects**

Hierarchic Model Structure

- Models to be Organized in a Top-Down Structure
  - Top Structure is Whole Reactor Level
  - Next Lower Structure is to be Local Zone
  - Next Lower Structure is to be Macroscopic Physics-Specific
  - Next Lower Structure is to be Microscopic Physics-Specific
  - Next Lower structure to be First Principles-Based Models
- Models to be Linked to Provide Local Virtual sub-Regions of the Reactor(s)
- Sub-Regions and their Models to be Mapped to the Computer Architecture

Full-Reactor Transport Theory

- Provides High Fidelity Modeling of Neutronic Behavior
- Could be Monte Carlo or Deterministic Model
- Must be very FAST
- Must be able to Incorporate Detailed Treatment/Preparation of the Cross Sections
- Must be Amenable to Implementation on Modern Computer Architectures
- Must Allow Feedback and the treatment of depletion/isotopics (with varying levels of detail)
- Must be Amenable to Time-Dependent Models Building

Thermal-Hydraulics Coupling

- Must be Capable of Treating a Variety of Coolants
- Must preferably avoid ad-hoc, empirical correlations that apply only in pre-determined regimes
- Could use Correlations Derived/Computed online in next Lower (deeper) level of Hierarchy based on First Principles
- Must be Tightly Coupled to Neutronics in a Multi-Physics type of Approach
- Must include steady-state and transient capabilities
- Must be very FAST

Nuclear Data Integration

- Cross section data and feedback therein
- Must be available and possibly processed and modified online (in lower level of computational model hierarchy)
- Resonance treatment must be explicit and involve continuous energy modeling of massively large groups of energy
- Feedback must be included either pre-tabulated or computed online on demand
- Data must fully reflect the spectral conditions in each sub-zone and must swiftly adapt to changes in said conditions

First Principles-Based Feedback Phenomena and Related Effects

- **Temperature Feedback**
- **Materials Feedback Effects**
  - **Thermal Scattering and Thermalization**
  - **Multi-Scale Phenomena: from the single atom to k_{eff} in damaged and undamaged materials**
  - **Radiation Damage and Annealing: Implications for safety Performance of Reactor**
- **Fuel/Core Reconfiguration Effects**

Design and Optimization Tools

- Nuclear systems are very complex: large number of degrees of freedom for optimization
- Mathematical optimization can result in higher confidence that optimum design decisions within constraints are being made
  - Reduction in system costs
  - Facilitating comparative studies of alternative systems
- Engineering time can be reduced
- Considerable computational resources are required to span the decision space to locate optimum and feasible solutions
- Commercial nuclear industry does have extensive experience in using mathematical optimization
  - LWR core design
  - Limited experience for other applications

Data Uncertainty Propagation and Design Margins

- Design margins must be introduced to account for data and model introduced uncertainties
- Design margins increase the system's cost, e.g. operate at lower power level
- Quantification of margins will indicate where additional efforts to reduce margins are economically justified
- Data uncertainties
  - ENDF/B covariance matrices
  - Propagating micro data uncertainties to macro system performance attributes uncertainties is computational intensive
- Modeling uncertainties
  - Model assumptions and discretization errors → higher fidelity models
  - Determining reasonable upper bounds is challenging
- Substantial computational resources are required to complete sensitivity and uncertainty analysis

Integration of Virtual Reactor Model Within Exploitation Shells

- Standalone for initial design and “final” prototyping
- Within Genetic Algorithm/AI decision Aid for Optimization Applications and Design Refinement
- Dynamic interface(s) for Simulation Applications
  - What if there is an earthquake?
  - What if we load a different fuel composition at some location/
  - Etc …
- Virtual Reality Environment for Training
- Etc …

Challenges: Computational Intensity and Models Complexity

- Models are expected to be very complex
- Complexity increases with lower (deeper) model in hierarchy
- Computational intensity (processor speed, memory requirements) increase as higher fidelity is sought with increasingly deeper models within the hierarchy
- Computer desired will have an architecture with a mix of shared and distributed memory and will have a large number of groups of processors
  - A group of processor could be dedicated to a sub-region of the reactor with all levels of the hierarchy of models represented in each group of processors
- Inter-region communication should be fast and would take advantage of the shared memory

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Is this Feasible?

- At INL, NC State, and elsewhere, portions of a "Virtual Reactor Model" are now being worked on, and have been before.
- Recent developments in the underlying sciences and methods have resulted in a situation where first-principle models are now possible, though not always routine
- Lack of access to proper computers has severely limited progress in many instances in which validity of approach has already been established

Is this desirable?
What science content?

- Each of the underlying components involves the development of advances in computational methods
- Each involves development of new science and physical understanding, though to varying degrees (some with quite substantial new insights)
- A high fidelity design and safety analysis tools will enhance the processes currently used to seek new technology
- A high fidelity design tool will result in costs savings and in better approaching/meeting design objectives (e.g. nonproliferation)

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Overview of Other Talks

- Gehin: Advanced Neutronic Simulation Development and Direction
- Rahnema: Zone-Mapped Approach to Full Reactor Neutron Transport Theory
- Haghighat: Massively Parallel Full-Core Transport Theory Methods
- Adams: Various Virtual-Reactor Challenges
- Hawari: the Neutronics-Materials Interface in Reactor Physics
- Thermal-Hydraulics, Multi-Physics, Materials of Interest to this Theme are Present Under other Groups.